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AN UNCERTAINTY INVENTORY DEMONSTRATION—A PRIMARY STEP IN UNCERTAINTY QUANTIFICATION

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Intended for:

11th AIAA Non-Deterministic Approaches (NDA) Conference, Palm Springs, CA, May 4-7, 2009



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An Uncertainty Inventory Demonstration—A Primary **Step in Uncertainty Quantification**

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Abstract

Tools, methods, and theories for assessing and quantifying uncertainties vary by application. Uncertainty quantification tasks have unique desiderata and circumstances. To realistically assess uncertainty requires the engineer/scientist to specify mathematical models, the physical phenomena of interest, and the theory or framework for assessments. For example, Probabilistic Risk Assessment (PRA) specifically identifies uncertainties using probability theory, and therefore, PRA's lack formal procedures for quantifying uncertainties that are not probabilistic. The Phenomena Identification and Ranking Technique (PIRT) proceeds by ranking phenomena using scoring criteria that results in linguistic descriptors, such as importance ranked with words, "High/Medium/Low." The use of words allows PIRT to be flexible, but the analysis may then be difficult to combine with other uncertainty theories. We propose that a necessary step for the development of a procedure or protocol for uncertainty quantification (UQ) is the application of an Uncertainty Inventory. An Uncertainty Inventory should be considered and performed in the earliest stages of UQ.

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I. Introduction

We have adopted the following operational definition:

Uncertainty Inventory is an organized set of all the information, statements, and questions relating to the different kinds of uncertainties in a given problem/application. The Uncertainty Inventory includes choices, such as which uncertainty mathematical theory(ies) is (are) appropriate for characterizing each uncertainty, and what data/information/knowledge characterize each uncertainty. The format of the Uncertainty Inventory could range in complexity from a list or table, to an interactive, relational knowledge base.

The above definition refers to different kinds of uncertainties. Examples of these are:

- Physically random error or aleatoric or irreducible uncertainty
- Probabilistic uncertainty (uncertainty of outcome of event)
- Prediction uncertainty (what is to be learned or inferred, what happens next, or what is the goal of an experiment)
- Scatter or dispersion in the data, or variance uncertainty
- Parameter uncertainty (from a model, including a chosen probability density function or PDF)
- Ambiguity uncertainty of physical cause or phenomena
- Threshold uncertainty (determining cut-off values, specifications, margins or boundary conditions)
- Statistical inference uncertainty (inferring information regarding the whole population from a sample or subset of observations, tests, or experiments)
- Vagueness of definitions, quality of science/scientist/environment
- Scaling, or scaled inference or similarity of phenomena uncertainty
- Model uncertainties due to assumptions, simplifications, model-form
- Epistemic or lack-of-knowledge uncertainty
- Linguistic uncertainty (e.g. do physicists and engineers use the same vocabulary)
- Measurement or instrument uncertainty (e.g. which is the target of investigation, which is the diagnostic, which are the driving forces, which is the recording device)
- Model parameter uncertainty (includes computer models, model-form uncertainty, physical, statistical, and mathematical models, operator-split models)
- Misclassification uncertainty (e.g., Zadeh fuzzy sets)
- Imprecision and inaccuracy uncertainty
- Non-specificity uncertainty (arising from lack of specific information).

Some authors, (e.g. Ayyub and McCuen, 1997) assert that uncertainties in engineering systems can be categorized according to whether or not they are mind-based abstractions of reality. We have found that such sub-categorization of uncertainties is not entirely helpful, but the practical goal of considering which mathematical theories are relevant is helpful. The uncertainty inventory serves several purposes and goals:

Provides a traceable, updatable record of the UQ

- Provides the seed of a protocol; adherence to protocol establishes scientific quality and experimental quality, such as reproducibility
- Permits different levels of information content, e.g., coarse versus detail, systemlevel versus component, complex-structure versus simplified
- Aids in determining the nature of the Total Uncertainty (see Ross, 2003) for the problem
- Provides the information necessary for decision making, certification, validation, risk/reliability estimation and other assessment conclusions
- Accommodates multiple quantities of interest, their predictor variables, and other ancillary quantities—a multivariate structure
- Permits numeric quantities, ordinal quantities, and even qualitative information (e.g., linguistic information)
- Aids in determining which uncertainties are the most influential on the answer and, hence, which are worth the cost to obtain more data/information for uncertainty reduction
- Provides a "learn by doing" environment, where weaknesses and strengths can be identified in the UQ process
- 10. Becomes a resource of knowledge and information that can evolve as new information becomes available or as things change. The person evaluating uncertainty should not need to be expert in both (for example) statistics and computational fluid dynamics, but be facile in how these topics are *interacting*.

Item 3 refers to the content of information contained within the recorded material in the inventory. Continuous variables, measurements, quantities, responses, have the most information content and have the highest quality. The minimum information content is captured with words. Words (linguistics) have the greatest flexibility, but can be the most difficult to analyze. While scientific practitioners prefer to have numeric data from tests, experiments or observation, there is valuable information content in the linguistic information recorded from observation or experience. When tests become too difficult or expensive (or illegal) to perform, the practitioner must take advantage of all available information, including that contained in expert's statements.

Information content can be ordinal (ordered) in nature, as part of quantification. Traffic light colors indicating ordering of good (green), medium (yellow) and bad (red) are commonly used (e.g., Zang et al., 2008). The *Phenomena Identification and Ranking Technique* (PIRT) *importance* is often rated using a three-level ordinal scale of High (H), Medium (M) and Low (L), and the *knowledge level* is rated using Known (K), partially known (P) and Unknown (U) (Diamond, 2006).

In addition to the form of the information (numbers versus words), the resolution or granularity of the information is also important in determining uncertainties and doing analysis. For example, in reliability assessment, counting the number of successes or failures is a coarser quantification than measuring quantities relating to failures such as strain. The courser counting can mask subtle details of the failure mechanics, and it presumes that we can "define failure", (e.g., Wahl, I., 2006) which is the subject of considerable ambiguity.

Item 9 is a common benefit of Probabilistic Risk Analysis (PRA). The remaining items relate to the benefits of having an inventory.

To achieve these goal and benefit of uncertainty quantification, a thorough, logical and organized effort is required for determining the fundamental elements of an uncertainty inventory.

Some examples follow:

- A. Source(s) of Inference Uncertainty (IU): are the observed phenomena the same, similar, or different than what is desired to be known? The answer to this question often involves making an inference, with attendant uncertainty (Langenbrunner et al. 2008).
- B. Which theory(ies) are applicable for the quantification of the uncertainty and to what degree are they applicable (see GIT list below)? For example, an experimental data set may be sparse, with a sample size of less than approximately 30.
- C. Which assumptions and/or conditions and/or caveats are required or necessary to interpret an experiment, to interpret simulation results (e.g. which assumptions involve model-form uncertainty)?
- D. Validation of a computer code may invoke uncertainty by affecting accuracy (bias or off-target center) or precision (wide or narrow scatter). Validation experiments may involve uncertain diagnostic dynamic range, bandwidth, or all of the above.
- E. Does categorization of uncertainty into reducible or irreducible components help the researcher? Does more knowledge, data, theory, information reduce the uncertainty in a computer code, or in an experiment?
- F. What is the name or type of uncertainty, e.g., is precision confused with accuracv?
- G. Does the relative importance for solutions change with time (e.g., traffic light or PIRT scale). Is the initial assessment evolving with respect to other elements, or with additional data, models and simulations?
- H. What level of quantification is possible; are the observables continuous numeric, ordinal, or qualitative only?
- I. Does necessary data or information exist (expertise, tests, observables, calculations, history)?
- J. Which data, calculations, models, simulations and variables may become available later?
- K. Do similar applications (or historical application) with data and/or calculations exist? Can these applications be applied to the present problem?

There are many mathematical theories that may provide appropriate characterization of the different kinds of uncertainties listed above, and these should be considered and tabulated as part of the Uncertainty Inventory. These theories can be collectively referred to using the title from George Klir's book (1998), General Information Theories or GIT. A partial list of uncertainty quantification techniques includes:

- Probability Theory (PT)
- Zadeh Fuzzy Sets and Logic Theory (ZF)
- Possibility Theory (POST)
- Dempster-Shafer Evidence Theory (DS)
- Imprecise Probability Theory (IPT)
- Random Intervals (RI)
- Concentration-of-measure inequalities (COM), (Lucas et al., 2008)

II. Granularity and Vagueness in Expert Elicitation

Before proceeding to the notional example sections that illustrate the construction and value of an uncertainty inventory, we reflect on importance of the use of expert elicitation for PIRT scales. PIRT scales call attention to one of the above GITs, Zadeh fuzzy sets (ZF) (Zadeh, 1965). In elicitation, Meyer & Booker (2001) found that technical/professional experts are comfortable with using a continuous scale compared to a discrete scale, such as the traffic light H, M, L or K, P, U scales in PIRT (e.g., Diamond, 2006). Figure 1 shows such a scale used in their studies, accompanied by the traffic-light gradient where green is Low, yellow is Medium and red is High. The scale in Figure 1 is listed as a numeric percentage, but this could have been labeled using an ordinal scale where the left end represents no importance and the right end represents complete or highest importance. The choice of labels depends upon the phenomena being considered and the community of practice of the experts. Community of practice is a term from Quinn and Holland (1987), referring to people's customs, artifacts, oral traditions, what they know to act as they do, and how they interpret their experience in a distinctive way. Most scientists and engineers are numerical thinkers and prefer a number line. However, there are some cases (e.g., using the seismic scale) where a log or order of magnitude scale is appropriate because that coincides with how the experts think.



Figure 1. Continuous PIRT importance scale as an alternative to H, M, and L sets.

Presenting experts with a continuous line, ordinal or numeric, and asking them to mark their answer (along with an uncertainty range) gives them flexibility and produces a finer level of detail in their answers. Recall that understanding the granularity, coarseness or level of detail is a key featured item in the uncertainty inventory. The continuous scale can be regarded as a *crisp solution*, because it avoids the *fuzzy* boundaries between

the discrete sets of H, M and L. An expert or decision maker may not want to crisply classify their answers into just those three choices (or sets), preferring instead some mixture in-between them. Such difficulty in deciding where the boundaries are between the 3 choices, or *fuzziness*, is the uncertainty due to classification and emerges from the limited choices presented (in this case H, M or L) and/or from a lack of definition associated with those choices. The continuous scale avoids the difficulty of deciding between a limited number of choices, especially if exact, precise definitions among the choices are not provided or practical. The uncertainty caused by the lack of good definitions can be reduced to a negligible level by providing them. The uncertainty of classification is more of a problem for some experts than for others. Bias is induced when the expert having this problem is forced to choose only one of the three answers.

Figure 2 shows how three different experts would use the continuous importance scale in PIRT. Their estimates are listed with A, B, and C. Experts were also asked to provide a range along with their answer, and these ranges are in the brackets.

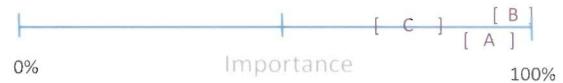


Figure 2. Three experts provided answers A, B, and C along with ranges (in brackets) on the continuous importance scale in PIRT.

In constructing an uncertainty inventory, one would want to include the uncertainty in the brackets provided by the experts. That uncertainty in the experts' minds about what the value of importance should be could be characterized using PT, POST, RI or IPT. Another alternative to using the continuous line using ZF follows.

Whenever linguistic terms are used as a response, like H, M, L, the uncertainty of classification emerges. There may be no exact interpretation of H, M, and L in a PIRT evaluation, making this a prime example for the use of fuzzy *membership functions*. When a PIRT decision is made to label a phenomenon as either H, M or L, especially in a Probabilistic Risk Analysis (PRA), there is no option to decide on something inbetween those three. Zadeh fuzzy sets (1965), allows one to quantify supplied responses (descriptions) like:

Expert A: "Well, this is mostly H, and little bit M."

Expert B: "This is definitely an H."

Expert C: "Gads, this is somewhat H and somewhat M. I cannot decide which."

Fuzzy membership functions are designed to handle these kinds of statements from experts. Figure 3 shows a simple construction of membership functions for the fuzzy sets of H, M, and L.

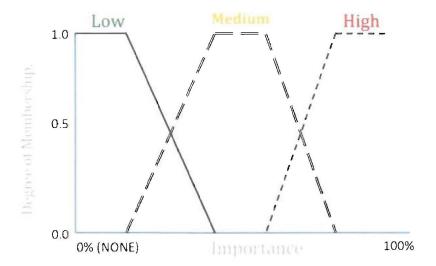


Figure 3. Membership functions of importance fuzzy sets for L, M, and H.

Instead of the three experts providing their answers and ranges on the continuous line in Figure 2, they use the fuzzy membership functions and indicate where their answers lie. The vertical lines in Figure 4 indicate their choices. The degree of membership in the three fuzzy sets for each expert is given in Table 1.

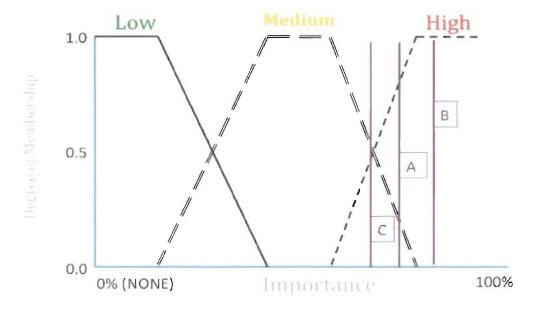


Figure 4. Three experts quantifying their linguistic statements using fuzzy membership functions for importance.

Table 1. Degree of membership in each fuzzy set for three experts

EXPERT	μн	μм	μι
А	0.8	0.2	0.0
В	1.0	0.0	0.0
С	0.5	0.5	0.0

The uncertainty in classifying their responses among the three choices of H, M, and L is now quantified in the degree of membership in Table 1.

Description of ZF and its uses are beyond the scope of this paper, however the use of scales during expert elicitation illustrates how easily the uncertainty of classification can emerge in the most common situations, i.e., using a PIRT scale. It also shows how easily sources of uncertainty can be discovered when performing an uncertainty inventory.

III. Notional Example: Explosive causing failure in-flight

We have created a simplified example to demonstrate an uncertainty inventory, in the form of a list. The objective of the notional example is to aid the decision maker to make decisions regarding how the airline industry can prevent passengers from taking explosives on board. In this example, the path forward is decided that the scientist/engineers (experts) quantify the amount of explosive which must be detected (or a lower value for the threshold-for-detection) before passengers board an aircraft. The experts begin by analyzing the consequence of explosions, specifically that which causes airplane failure in-flight. How shall the experts then quantify the uncertainty in this problem? This problem is not entirely suited to a PRA because of the lack of knowledge and sparseness of data, the difficulty (ambiguity) of determining threshold values for amount of explosives needed to cause different degrees of damage, the heavy reliance on expert knowledge in linguistic form, the inability of most computational codes to model complex boundary conditions, the poorly known behavior of heterogeneous material properties under dynamic, three-dimensional states of loading, and the non-specificity in defining such states as "failure", or "severe damage" or "safe"

One powerful tool in use by the Nuclear Regulatory Commission (NRC) for uncertainty quantification is the Phenomena Identification and Ranking Technique (PIRT). It is a method that can be used to identify important parameters in a problem (including computer model parameters) to support a specific decision objective. The methodology is meant to identify all phenomena, as well as rank the most important, using the process of expert elicitation (Meyer and Booker, 2001). If a phenomenon is identified as being important, it is also ranked for its corresponding knowledge level. For example, if

a phenomenon is ranked with "High (H)" importance and knowledge is "Partial (P)" or "Uncertain (U)", then, the Nuclear Regulatory Commission has determined the simultaneous presence of these criteria warrants research, as in the table below, (Diamond, 2006). If the phenomenon is known (K), research is not necessarily warranted.

Table 2. as in Diamond (2006).

Phenomenon	Importance High (H)	Importance Medium (M)	Importance Low (L)
Knowledge level K	No research	No research	No research
Knowledge level P	More research	No research	No research
Knowledge level U	More research	More research	No research

In this notional example, it is decided that one objective is to determine the smallest amount of explosive detonated inside an aircraft that will cause catastrophic damage. The uncertainty inventory process starts by listing phenomena that affect the desired result (catastrophic damage measure). The phenomena can be assumptions, parameters, boundary conditions etc. Rivet and material failure models in the aircraft simulation are two relevant examples.

In the case of a phenomena that is considered to have high importance, but partial knowledge, (e.g. failure criterion in Table 3 below), more research should be conducted and resources invested to reduce the uncertainty and thus obtain reduced uncertainty in the result. If more research cannot be done, the next step is to quantify our knowledge of uncertainty, in lieu of gathering more experiments or simulation-based data. For example, certain types of testing may be illegal or undesirable or impossible, such as full-scale testing of nuclear weapons, full-scale test of a building during an actual earthquake, or full-scale testing of explosives during flight.

Depending on the type of uncertainty, expert knowledge can be compiled or computer model simulation results can be analyzed to rate the level of importance for each phenomenon. The level of uncertainty can be based on expert knowledge or can be expressed as a mean and standard deviation (we are using PT at this point) derived from model runs, where the model input uncertainty is propagated through the model. In order to more fully understand the process, an example uncertainty inventory table is shown below. Table 3 is analogous to the many techniques used in enumerating and assessing risks and/or failures in PRA and PIRT. This idea of organization is not new, but the information contained in the columns and rows is new, because it is designed for an uncertainty inventory.

The uncertainty inventory for our notional example includes a column for phenomena and uncertainty sources, a column for an appropriate uncertainty theory, a column for a

proposed approach to the uncertainty, and a column each for importance / uncertainty level. The appropriate uncertainty theory or approach may include Expert Knowledge, (EK), Calculation-to-Calculation comparison (C-C), Calculation to Experiment comparison, (C-E), or Experiment-to-Experiment (E-E) comparison. Note that the column for Knowledge Level has in its designation a measure of its uncertainty. The Importance level may be uncertain as well, and a column could be incorporated to capture that uncertainty. The key to the abbreviations in the column for "level of quantification possible" is CN (Continuous Numeric); QO (Qualitative Ordering).

Table 3. Notional Example Uncertainty Inventory (Explosive detonated in an Aircraft)

Phenomenon or Source of Uncertainty	Appropriate uncertainty class or Mathematical theory	Approach (EK), (C-C), (C-E)	Knowledge	Relative Importance (H, M, L)	Level of Quantification Possible
Symmetry effects, 3-D effects	Ambiguity, POST	EK, C-C	Р	M	QO/CN
Boundary conditions (Simulation)	Vagueness, IPT	EK, C-C	P	M	QO/CN
Failure criterion	IU, Ambiguity, ZF	EK	P	H	QO
Yield / hardening material model	Ambiguity, ZF, PT	EK	K	M	QO/CN
Physics not modeled	POST, PT, IPT, ZF	EK, C-C	U	M	QO/CN
Measurement Error	PT	C-E	P	M	CN
Device Variability	IPT, ZF	C-E	P	Н	QO/CN
Modeling parameters	Ambiguity, PT, IPT	EK, C-C	K	M	CN
Failure behavior in fracture	Vagueness, POST	EK, C-E	P	L	QO/CN
Explosive types	IU, ZF, PT	E-E, C-C	P	M	QO/CN
Similarity w/ historical events	PT, IPT, POST, ZF	C-C	P	Н	QO/CN
Flight loads	Vagueness, ZF	EK, C-C	P	Н	QO/CN
Temperature effect	IU, Ambiguity	EK	K	L	CN
Strain rate effect	Ambiguity, IPT	EK, C-C	P	M	QO/CN
Mismatch of Data w/ Calculation	IU, Ambiguity, IPT	EK, C-E	P	Н	QO/CN

For example, there is IU when the desired quantity is the explosive effect on the passengers in the airplane. Detailed knowledge of how human passengers are affected by such an explosion could presumably make the issue of airplane damage moot. This uncertainty includes the inference uncertainty of testing explosive effects on humans compared to animals, an uncertainty shared in common with the prescriptive drug industry. There exists data for similar applications, however, such as the effects of explosives on humans in the confines of military vehicles. Using that data would introduce "inference of similarity" uncertainty. Table 3 is analogous to the many techniques used in enumerating and assessing risks and/or failures in PRA and PIRT. Additionally, knowledge of uncertainty can be integrated, using expert elicitation, and other techniques, as indicated below. The reader should keep in mind that inventories change, and Table 3 is meant as a notional example, only.

IV. Quantifying Uncertainty for Notional Example of Explosive causing failure in-flight

It is evident from Table 3 that a key feature in quantifying and reducing the uncertainties in the notional example is the appropriate use of expert knowledge (EK). There exists modeling expertise, explosive expertise and aeronautics expertise, but few experts employ experience in all of these areas simultaneously. This is because there is sparse data for explosives detonating in-flight on civilian airlines. We submit that this restricts the application of Probability Theory (PT) or a PRA for this example, unless there would be a method of casting the inference uncertainty into PT. How then can the uncertainty inventory in Table 3 aid the decision maker, or the engineer/scientist?

Knowledge from expertise and experience within a single field can provide judgments needed for a sparse-data problem. For example, an explosives expert is clearly relevant in our notional example, even if they have no aeronautics experience. Such an expert can make a quantitative assessment of prediction errors of an explosives computer code. What we are describing is the collection and utilization of all sources of data and information to aid in quantification of uncertainties, especially for data-sparse examples. We call this process *Information Integration*, (Booker, Bement, Meyer, Kerscher, 2003) and it begins by accumulating the information from all the sources for organization in a knowledge base. An uncertainty inventory is an example of the knowledge base.

Langenbrunner, Booker, Hemez, and Ross (2008), using a "4-box approach", made a simple demonstration of the information integration technique. The notional example, using the 4-box techniques can be illustrated in Figure 5. Those authors combined several types of uncertainty using expert elicitation. The top row of boxes represent physically-relevant experimental data, the green box represents physics-validation experiments, the red box represents actual airplanes-in-flight with explosive events. The bottom row of boxes represents code calculations or simulations. The blue box represents small-scale simulations, producing probability of failure. Failure is defined by criteria applied to the output the simulations, in terms of a threshold of one or many terms. The gold box represents full-scale airplane simulations.

The boxes on the left are called "data-rich" and those on the right are "data-sparse." The contents of boxes on the right-hand side of Figure 5 can be likened to the phenomena and uncertainty sources in Table 3. The physics experiments data box (green) and the full-scale explosions data box (red) can contain similar data, except that the physics experiments are routine or data-rich, and the full-scale airplane data are sparse. The example shown in Figure 5 assumes that the small-scale tests are a data-rich application and the full-scale explosions represent a data-sparse application. The 4-box technique constitutes construction of the knowledge base, just as does the uncertainty inventory.

By considering the full-scale explosions alone, uncertainties in failure criteria may be unnecessarily inflated because of inference uncertainty. By considering the small-scale experiments alone, the failure criteria may be too narrow. Scaling constants, from small-scale to full-scale experiments can be difficult to determine. The observables have

measurement errors. The functional forms of models may admit additional inference uncertainty. These issues are part of the uncertainty inventory.

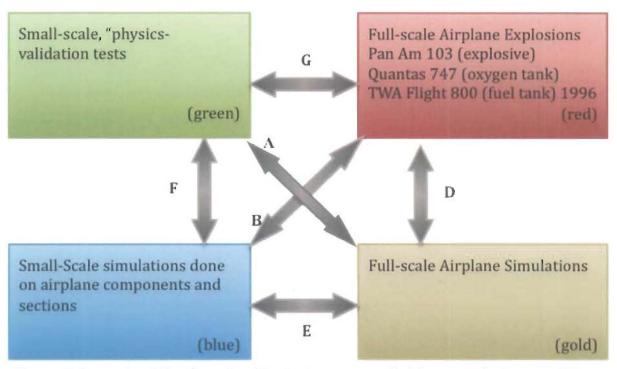


Figure 5, Example of the "four-box" technique, as applied to an explosive event in an airplane example.

Table 4. Comparisons between two applications for tests and codes (see Fig. 5).

Arrow	Type of Comparison	Comparison Conveys Information About:
А	Calc-to-Expt. (C-E)	Common modeling and/or bad observables
В	Calc-to-Expt (C-E)	Common modeling
D	Calc-to-Expt (C-E)	Physics or theory not modeled
E	Calc-to-Calc (C-C)	Common physics modeled
F	Calc-to-Expt (C-E)	Physics or theory not modeled
G	Exptto-Expt (E-E)	Repeatability through similarity

Returning to the uncertainty inventory, the reader will note that the column designated "Approach" has Calculation-to-Calculation comparison (C-C), Calculation to Experiment comparison, (C-E), or Experiment-to-Experiment (E-E). These comparisons can be seen in the 4-box technique in Figure 5 indicated by the double-sided arrows. The experiments (boxes in the top row) have physics in common denoted by arrow G. The two boxes in the bottom row have computer code models in common denoted by arrow E. A simplistic summary of the arrows is listed in Table 4.

One way to quantify these comparisons is to apply a goodness-of-fit metric of test-analysis correlation (e.g., the D_N metric, Langenbrunner, Booker, Hemez, Ross, 2007) to the observables. This particular metric permits the specification of three kinds of uncertainties which can be expressed as variances (using PT). Another way to quantify these comparisons is to establish a scoring scheme based upon counting the degree of and nature of similarities. These techniques are the subjects of future research.

V. Summary

The authors have given an operational definition of an Uncertainty Inventory, and offered a notional example. An Uncertainty Inventory is a set of all the statements that are questions relating to uncertainty. The Uncertainty Inventory is a part of the knowledge base of problems in uncertainty quantification. Part of the inventory is an assessment of what uncertainty mathematical theory appears most appropriate, and/or an approach to quantifying the uncertainty. Expert knowledge can be used to quantify uncertainties of differing types. One method, the 4-box technique, can help organize pair-wise comparisons of uncertainties in phenomena. This is important for scenarios where decisions must be made under severe uncertainty about data-sparse applications.

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